REMARKS

Claims 5-16 and 19-27 are pending in the above-identified application. Claims 5-16 and 19-21 stand rejected under 35 U.S.C. §§ 102(a) and/or 103(a). Claims 22-27 stand rejected under 35 U.S.C. § 112, first paragraph. Applicant respectfully requests reconsideration of the claims in light of the amendments and remarks made in this response.

With this amendment, claims 5, 9-12, 20, and 21 have amended. Claims 7 and 22-27 have been canceled. Claims 28 and 29 have been added. These amendments are made without prejudice as to further prosecution of the subject matter of precedent claims in continuing applications.

None of these amendments adds new matter. Support for new claims 28 and 29 is found throughout the application, in particular at page 8, lines 17 through page 9, line 2; page 12, lines 14-19; and page 23, lines 1-16. Their entry is respectfully requested.

I.   Rejection under 35 U.S.C. § 112

Claims 22-27 stand rejected under 35 U.S.C. § 112, first paragraph, as allegedly failing to comply with the written description requirement because they include new matter. Specifically, the Office Action contends that there is no support in the specification for the limitation "tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and backtracking the path when an inconsistency is detected." Applicant respectfully disagrees.

As an initial matter, Applicant notes that, solely in an effort to expedite prosecution of the remaining claims, claims 22-27 have been canceled. Nevertheless, because the limitations in these claims have been included in the independent claims, Applicant addresses this rejection below.

The Office Action states that the claims do not specify the position in the traced path to which the backtracking falls back. Applicant submits that the specification teaches how to perform the appropriate backtracking and that amendment of the claims to specify such is not required. Nevertheless, the independent claims have been amended to specify that the path is

-8-

backtracked "to the last assignment that was made." Support for this amendment is found in Figure 22 (step 1060) and pages 11-13 of the specification. Applicant submits that this amendment is fully supported by the specification.

The Office Action also states that the claims "generically recite[] backtracking when an inconsistency is detected" and that there is no definition or teaching regarding the term "inconsistency." Applicant believes that a person of skill in the art would understand the meaning of the term "inconsistency" in light of the claims and the specification. Nevertheless, the independent claims have been amended to state that backtracking occurs "when an unacceptable state is detected." Support for this amendment is found in at Figure 22 and page 12, lines 5-9 of the specification. At page 12, the specification provides an example of an unacceptable state (an oxygen atom having one double bond and one uncharacterized bond). The example further explains that the electronic state and valence distribution information is used to determine if an unacceptable state is found. Applicant submits that this information provides support for the amended claims. Moreover, this teaching, along with the teaching of the specification as a whole, would allow a person of skill in the art to practice the invention without undue experimentation.

The Office Action further states that the specification does not support generically assigning bond order and atomic charge as the path is traced and indicates that the claims must include a limitation drawn to assigning an ESVD to be supported by the specification. Applicant strenuously objects and submits that the claims are supported by the specification. As the Office Action notes, the specification at page 5, lines 8-12 electronic and bonding state is examined for each possible structure. Moreover, pages 6-7 provide further teaching about how bond orders and atomic charges may be assigned. Specifically, the example of using electronic state and valence information is provided at these pages. As explained at page 6, lines 10-11, the atomic environment includes "a charge or an unpaired electron or both, in addition to bonding information. The collection of characteristics involved is referred to hereinafter as an environment _or_ as an electronic state and valence distribution." Thus, the specification does not limit assignment of bond orders and atomic charges/radicals to the particular embodiment of

using an ESVD. Applicant submits that, as filed, the specification supports the limitation "assigning bond orders and atomic charges or radicals."

For the foregoing reasons, Applicant submits that the amended claims are fully supported by the specification. Accordingly, Applicant requests that this rejection be withdrawn.

II.   Glendening and Graovac Rejections

Claims 5-16 and 19-21 have been rejected under 35 U.S.C. § 102(a) as allegedly being anticipated by Glendening *et al.* Claims 5, 11, 15, and 20 have been rejected under 35 U.S.C. § 103(a) as allegedly being obvious over Graovac *et al.*

Solely in an effort to expedite prosecution of the remaining claims, independent claims 5, 9, 10, 12, 20, and 21 have been amended to incorporate the limitations of claims 22-27, respectively. As claims 22-27 have not been rejected in view of Glendening *et al.* or Graovac *et al.*, this amendment is rendered moot as these references do not teach all of the limitations in the amended claims, either alone or in combination. Specifically, neither Glendening nor Graovac teach a method that includes tracing a path through the structure, assigning bond orders and atomic charges or radicals as the path is traced, and, when an unacceptable state is detected, backtracking the path to the last assignment that was made. Thus, Applicant submits that the claims are novel in view of Glendening and Graovac. Accordingly, Applicant requests that this rejection be withdrawn.

III.   Substantial Claim Duplication

The Office Action objects to claims 7 and 8 under 37 C.F.R. § 1.75 as being substantially duplicative. With this amendment, claim 7 has been deleted, rendering this objection moot.
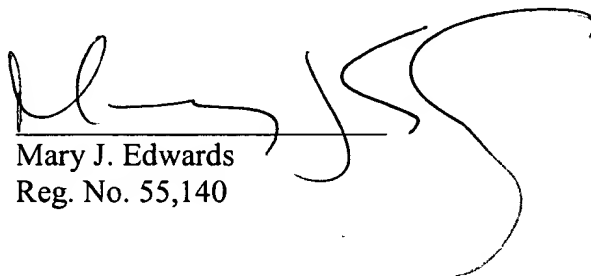
IV.   Conclusion

In view of the foregoing remarks, Applicant submits that all pending claims are in condition for allowance, which action is earnestly solicited.

Applicant respectfully requests an early and favorable reconsideration and issuance of this application as amended herein. The Examiner is encouraged to contact the undersigned to expedite prosecution of this application.

Applicant also includes a request for continued examination and a petition for a two-month extension of time to extend the period for response up to and including August 16, 2006. An authorization to charge the associated small entity fees of $620.00 to our Deposit Account No. 08-0219 accompanies this response.

No other fees are believed to be due in connection with this submission. However, if any fees are due in connection with this application, please charge them to our Deposit Account No. 08-0219.

Respectfully submitted,

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-11-